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Fluidized Bed Reactor Modeling and Simulation with Aspen Plus

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Abstract:
Fluidized bed reactor is useful for heterogeneous (multiphase) reactions, separations, size enlargement, coating, and blending in chemical and pharmaceuticals industries. To develop a model and simulation of this reactor with advanced systems process engineering software (Aspen Plus). Aspen plus has the capability to simulate real factory performance, design improved plants, and intensify profitability in present plants. This modeling and simulation are applied Geldart B particle classification, GGC is used for particle size distribution function, Newton parameters for mass convergence, and Ergun equation is used for minimum fluidization velocity calculation and pressure drop through the fluidized bed reactor. Generally, most of the predictions model from Aspen plus is a reasonable agreement through the experimental results. Advantage of this investigation is used small quantity of bed particlesand identified their melting point temperature is above 340°C. This fluidized bed reactor model and simulation is functional for aluminum hydroxide decomposition reaction. The feed 275 kg/hr of Al(OH)3is converted into 169.6 kg/hr of aluminum oxide (Al2O3) and 89.9 kg/hr of water. A total mass conversion percent is 94.4% of aluminum hydroxide.

Keywords: Fluidized bed reactor, decomposition reaction, Al (OH)3, modeling, simulation, Aspen plus, Geldart Bclassification and minimum fluidized bed.

1. Introduction toAspen plus modeling and simulation of Al (OH)3decomposition Reaction:

Decomposition reaction of the aluminum hydroxide is converted into aluminum oxide and water throughout the fluidized bed reactor. The product of the decomposition reaction is alumina (aluminum oxide), this production is using for a different purpose (Hawraa K. 2020). Alumina (Al2O3) is brilliant ceramic oxide through widespread applications, including adsorbents, catalysts, microelectronics, chemicals, the aerospace industry, and other high-technology fields (Vishnu 2017). This published article has described the importance of aluminum oxide uses as inert biomaterials and a decomposable material, well-tolerated in the biological environment (Nicola Luigi 2015). Also, a significantly use to produce aluminum metal, as an abrasive due to its hardness and high melting point (D. Redaoui 2016).A chemical reaction mechanism is given:

2Al (OH)3□Al2O3 + 3H2O

The stoichiometric of a reaction mechanism above, tell us two moles of the aluminum hydroxide is converted into one mole of alumina and three moles of water.The rate of reaction is indicated by the first derivative equations. The experimental rate equation in a power law method for conversion of hydroxides

can be stated as:

$$-r_{Al(OH)_3} = k C_{Al(OH)_3} \quad \text{----------1}$$

A reaction rate constant (k) is calculated applying a power law kinetic expression:

$$k = k_0 T^n * \exp\left(-\frac{E_A}{2RT}\right) \quad \text{----------}$$

Where k_0 - pre-exponent, T - temperature, E_A- activation energy, R- universal gas constant. The reaction kinetics parameter was experimentally studied with X-ray diffractometer by (Ienwhei Chen 1989) and (Lawrence Candela 1986), these kinetics parameters are very important for modeling and simulation when the kinetic reactions take place in the fluidized bed reactor or unit operations systems (Jens F. 2017). The pre-exponent of rate constant (k0) is 0.39 and activation energy (EA) is 7253.384 Cal/mol are taken from the experimental work of Lawrence Candela, to use in the modeling and simulation of aluminum hydroxide decomposition.

The fluidized bed reactor is the multifunction unit operations in chemical and pharmaceutic industries (Xianbo Yu 2010). Some of the functions are biomass steam gasification, crack high molecule hydrocarbons to produced light hydrocarbon molecule, coating and blending pharmaceutics products (German G. Silva 2012) and (QitaiEri 2018) are details described. In the present work, a fluidized bed reactor is used for the decomposition of the aluminum hydroxide. Using an advanced system process engineering software (Aspen Plus) modeling and simulation for alumina (Al_2O_3) with maximum yield and a small amount of solid bed particle. Aspen plus is one of the computer-aided processes engineering open access and denoted by CAPE-Open (ZhenxingCai 2017). A chemical processes simulation software has an actual important influence proceeding chemical engineering product design and operations, which can be used on processing optimization operation conditions, eliminate experimental time consumption and energy saving.

Aspen Plus is a tool for modeling and simulation software packages commonly used in the industries currently(Juma H. 2019).With a given procedure design and a suitable choice of thermodynamics and the mathematical models to expect the performance of the processes. It gives correct modeling of thermodynamics properties and particularly important in the separation of real mixtures and has huge databases generate parameters (Yu, Wu et al. 2020). Aspen Plus is a commercial software process modeling tool for concrete design, optimization, and performance monitoring aimed at the synthetic substance, polymer, specialty chemicals, metals and minerals, and coal power industries. One of the greatest advantages of Aspen Plus already has the current databases for species and their pure, binary, and tertiary regressed parameters. It can also handle very complex processes, such as Multiple-column separation systems, reactors, heat exchangers, and pressure changer.

In this project, Aspen plus software is the main tool and method for modeling and simulation an aluminum hydroxide decomposition reaction. To predict the fluidized bed reactor geometry, processes variables, reaction kinetics parameters, conversion of desired product, and operable operations conditions.

2. Aspen Plus Setup for Fluidized Bed Reactor:

This modeling and simulation project work is briefly indicated the two main procedures in this software. The first one is called thermodynamics properties method, also known as sample preparation in the real world. And the second is process flowsheet simulation is known as unit operations selectionfor solid-fluid reaction take place in Fluidized bed reactor.

2.1 Thermodynamics physical properties method for Sample preparation:

During the opening the Aspen plus template, select a solid with metric solids, this template is help us boundary conditions set in the simulation part(R. Mansour 2015).Now the components specifications going to specify via component ID, type, component name and alias. For gas and liquid components specified under a type called conventional, while solids components specified called solid. In this product processes four major components are participated, as table-1 below show components specifications.

Component ID	**Type**	**Component name**	**Alias**
Alumi-01	Solid	Aluminum-Hydroxide-Amorphous	Al (OH)3-A
Alumi-02	Solid	Aluminum-Oxide-Alpha-Corundum	Al_2O_3
Air	Conventional	Air	Air
Water	Conventional	Water	H_2O

As a table-1 above identified the chemical components involved in the product, almost Aspen plus data bank used capital words rather than small letters.

After completed components specifications, then select the best methods specifications based on the component behavior (physical properties) of a production process given a project or problems to modeling and simulation. In this case, a table-2 below is summarized methods specifications for Aluminum oxide production process.

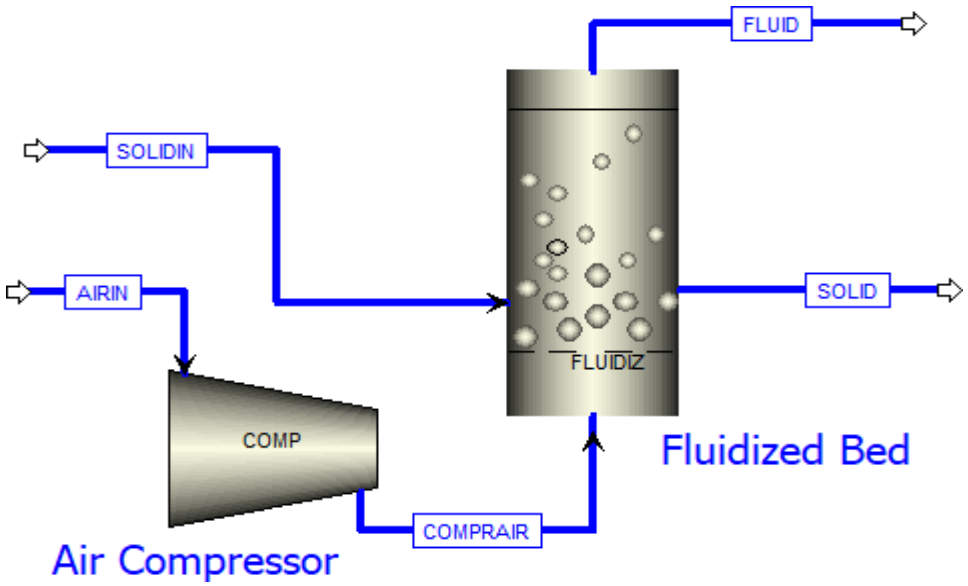
Methods Specifications			
Method filter is selected	ALL	method name is selected	SOLIDS
Base method is selected	SOLIDS		
Petroleum calculation options			
Free water method is selected	STEAMNBS		
Water solubility is selected	3		

Table-2 is detailed methods specifications selection ways for solid-liquid reactions product process, the caps locked words is the methods selected for this project work.

Consequently, completed the selection of components and methods specifications for sample preparations of a given project or problems. Thus, run a physical properties method orthermo dynamics methods (R. Barrera 2014). As Aspen plus response forran a wright physical properties analysis is calculations were completed normally.

2.2 Modeling and simulation for fluidized bed reactor and air compressor:

Throughout Aspen plus simulation opening the graphical user interface (GUI) is called main flow sheet. A main flow sheet window consists different unit operations and materials at a bottom or sometimes at a top tight in the folder of model palette. A figure-1 is represented the production process flow sheet for aluminum oxide.



From a figure-1, above give us the descriptions that consists two-unit operations, three inlet and three outlet streams. The unit operations require for this modeling and simulation is Air Compressor and Fluidized bed,a function of compressoris increasing the fluid pressure and a Fluidized bed, where the reactions and separations take place simultaneously.

2.2.1 Descriptions of Aspen plus Simulation Setup:

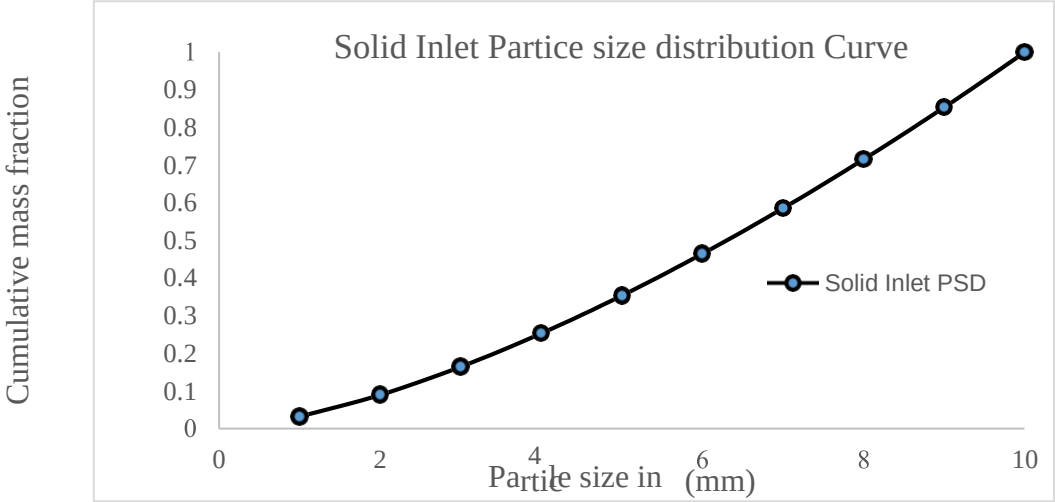
Start with flowsheet construct in main flowsheet or GUI, as figure 1 indicated. Careful checked the unit operations connect with streams (materials), the red arrays during the materials adding must be obligators as Aspen plus rule and regulation. A blue array uses for adding utilities, such as steam or coolant and etc. **Streams inlets:** Is one ofboundary conditions that the programmer identify the inlets of unit operations. A table-3 below is indicated a boundary conditions of inlets streams into air compressor and fluidized bed.

Stream name: Air in (into Air Compressor)				
State variables	**Amounts**	**Units**	**Composition in mass fraction**	
Temperature	25	°C	**Components**	**Value**
Pressure	1	bar	Al (OH)3	
Total flow basis	mass		Al2O3	
Total flow rate	4150	kg/hr	H2O	
			Air	1
Stream name: Solid in (into Fluidized)				
State variables	**CIPSD**	**units**	**Composition in mass fraction**	
Temperature	25	°C	**Components**	**Value**
Pressure	11	bar	Al (OH)3	1
Total flow basis	mass		Al2O3	
Total flow rate	275	kg/hr		

The important boundary conditions of a Fluidized bed are particle size distributions for the bed materials (D. Geldart 1998). Now this paragraph would be giving the basic concept of setup about particle size distribution (C. Montilla 2020). Open PSD mesh ID by down scroll PSD withunit millimeter (mm), make

active a distribution function under populate PSD using. Then choice a type of distribution function GGS, continue assign dispersion parameters 1.5 and maximum diameter 10mm, in this simulation.Where GGS is called Gates-Gaudin-Schuhmann, that is the general formula of distribution function for the cumulative distribution function(Candela 1986). A figure-2 is the particle inlet size distribution curve. Cumulative mass curve F(x) can obtain by means an integration of the frequency curve f(x) and respected to particle size dx.

$$F(x) = \int f(x)dx \quad ---------- \quad 3$$



This figure-2 is the results of populate particle size distribution by GGS model. This a model gives a plot cumulative mass fraction versus particle size, Aspen plus gives a plot above after input were completed and success on a calculate box icon. Thus, the particle size gives high yield of aluminum oxide product.

2.2.2 Operations Conditions of Air Compressor:

The air compressor is used to increases the pressure of air, that pressurized air is easy to pass through the bed material. A type of compressor is Isentropic, and outlet specifications is checked discharge pressure with 11 bar should be workable in this case.

2.2.3 Operations Conditions of Fluidized bed:

Many operations conditions need to specify for modeling and simulations of fluidized bed during use Aspen plus simulator software. Main operations conditions should be specified, like specifications of bed inventory, geometry of column, gas distributor, reactions and convergence.Convergence is the critical issue for modeling and simulation, after input completed running the modeling and simulation. If all boundary and operations conditions are satisfied (correct) the simulation should be convergence. That means, the results are available and ready for data analysis and discussions the results. This case mass balance convergence solver is used Newton parameters. While solver Broyden parameters not mass balance convergence.

In Aspen plus, the reaction setup is specified to open reactions folder at right side, create new reaction numbers with reactions type and stoichiometry. In this work the reactions setup specified as in a table-4 below indicated.

Stoichiometry specifications		
Rxn No.	Reaction type	Stoichiometry
1	Kinetic	2 Al (OH)3(CIPSD) □Al2O3 (CIPSD) + 3 H2O
Kinetic specifications		

Reacting phase =>Vapor		Rate Basis =>Reac (Vol)
Pre-exponent K0 value	0.39	
Activation Energy	7253.84	cal/mol

Bed particles specifications, geometry of column and gas distributor are summarized in a table-5 is described below. This operation conditions, during modeling and simulation of a fluidized bed should be requires input specified. A pre-exponent rate of constant and activation energy was taken from experimental published work by American Institute Chemical Engineers journal as book chapter(Candela 1986).

Specification			**Geometry of Column**		
parameters	value	units	parameter	value	unit
bed mass	50	kg	Height	2.5	m
voidage @min fluidization	0.5		Solid outlet	0.75	m
Geldart classification	Geldart B		Diameter	0.4	m
min. fluidization velocity	Ergunequations		**Gas Distributor**		
TDH model	George & Grace		type	perforated plate	
max. dC/dh	1.00E-05		number of orifices	40	
Elutriation model	Tasirin&Geldart		orifice diameter	10	mm

Whole, the boundary and operation conditions were input completed, now ready for run the modeling and simulations to obtain results for discussions and conclusion the project work. The Geldart class B particles start the bubbling fluidization process instantly reaching the smallest fluidization velocity(Semion Shaul 2014). So, these solid particles are used for bed particle material.

3. Results and Discussions:

Normally, afterward modeling and Simulation was run and converged, two results are available to discuss and analysis. Thus, results are unit operations and streams result summary. In this section detail descriptions of results through result summary and fluidized bed unit operations.

Results Summary: It consists run status, streams, convergence, operating costs, CO_2 emissions, streams (custom), models and equipment. Stream result is one of the result summaries, which consists theprocess variables and all streams are given in a table form.

As a decomposition reaction mechanism is given below, mass flow rate of aluminum hydroxide is 275kg/hr into a fluidized bed reactor. To remove water molecules from $Al(OH)_3$ used compressed air mass flow rate at 4150kg/hr with high pressure at 11 bar. This pressure is corresponded to temperature 422.8°C

$2Al(OH)_3 \square Al_2O_3 + 3H_2O$

The stream result table below is described all inputs and output after the modeling and simulation of project is converged. The amount of aluminum oxide is **169.6kg/hr**, and water is **89.9kg/hr,** are formed during the decomposition reaction take place; while **15.42kg/hr** aluminum hydroxide is remain.A table-6 is designated stream results from results summary.

Process variables	Air in	Comp Air	Solid in	Fluid out	Solid out
Temperature °C	25.0	422.8	25.0	338.8	338.8
Pressure bar	1.0	11.0	11.0	10.8	10.8

Mass VFrac	1.0	1.0	-	1.0	-
Mass SFrac	-	-	1.0	< 0.001	1.0
All Phases					
Mass Flow kg/hr	4,150.0	4,150.0	275.0	4,240.9	184.1
Volume Flow cum/hr	3,553.4	754.1	0.1	700.9	0.0
Enthalpy Gcal/hr	< 0.001	0.4	-1.1	0.0	-0.7
Density kg/cum	1.2	5.5	2,600.1	6.1	3,812.8
Mass Flow kg/hr					
Aluminum hydroxide			275.0	0.1	15.4
Alumina				0.9	168.7
Water				89.9	
Air	4,150.0	4,150.0		4,150.0	

The conversion of aluminum hydroxide is calculated from the simulation result presented in table above.

$$m_{a0}=\frac{m_{af}}{m_{a0}} * 100$$

where m_{a0} and $m_{af}$is mass flow rate of Al(OH)3inlet and outlet respectively. Hence, 94.4% mass percentage of aluminum hydroxide is converted into aluminum oxide and water.Based on this modeling and simulation results, possible to fix the property of solid particles (catalysis), which has a melting point temperature is greater than 340°C and resisted to broken at pressure 11bar. It is corresponding to operation conditions of the reactor.

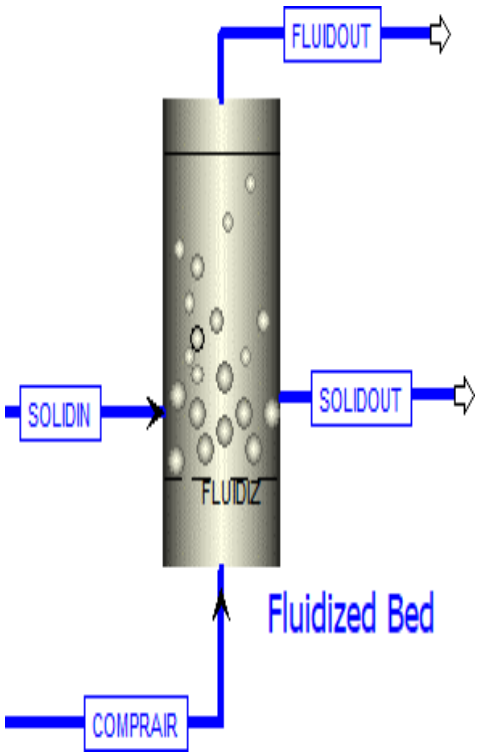
Unit operations (Fluidized Bed Reactor) Model results: From a given input parameters and selected equations models, Aspen plus is calculated the necessary process variables and parameter required for fluidized bed Reactor designD. Kunii (1991). The basic model equation is given as follow:

$$\Delta P = [\frac{150\mu U_{sf}}{*d^2}\frac{(1-\varepsilon)^2}{\varepsilon^3}+\frac{1.75\rho_f U^2_s}{\frac{f}{d}}*\frac{1-\varepsilon}{\varepsilon^3}]H------4$$

Equation 4 known as Ergun equation istelling to velocities lower than the minimum fluidization velocity besides considered as a packed bed state.

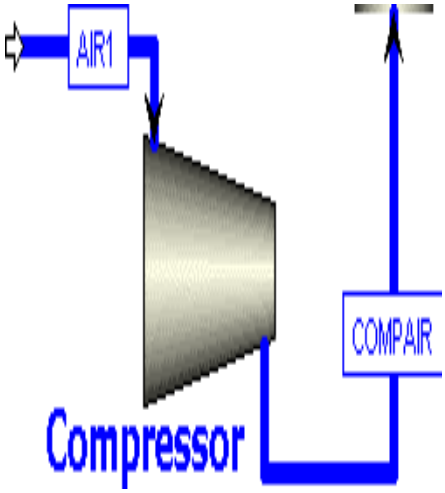
$$\Delta P = [(\rho_p - \rho_f)(1-\varepsilon)]gH - - - - - - - - - - - - - - - 5$$

Fundamentally, once the bed reaches minimum fluidization velocity the pressure drop is calculated fluidized bed state equation.A table-7 is indicated the summary of model results from Aspen plus.



Parameters and Process variables	Value
Height of bottom zone [meter]	0.089511457
Height of freeboard [meter]	2.41048854
TDH from correlation [meter]	2.23125858
TDH based on solids volume profile [meter]	2.41048854
Solids holdup [kg]	50.0001362
Number of particles in bed	5970160.15
Bed surface area [sqm]	20.2918358
Distributor pressure drop [bar]	0.19113425
Bottom zone pressure drops [bar]	0.008463783
Freeboard pressure drop [bar]	0.031979177
Fluidized bed pressure drops [bar]	0.04044296
Overall pressure drops [bar]	0.23157721
Heat duty [Gcal/hr]	0
Minimum fluidization velocity [m/sec]	0.724609882
Heat exchanger duty	
Bed temperature [°C]	338.845523
Moles generated from reaction [kmol/hr]	3.32676322

The model and simulation result are indicated in combination of figure and table above. Ergun model equation is used to calculate of minimum fluidization velocityand gives a modeling and simulation is converged. From a result table is obtained details specifications about fluidized bed reactor.Detail specifications of air compressor isobtained from the model and simulation result.



Compressor model	Isentropic Compressor
Phase calculations	Vapor phase calculation
Indicated horsepower [kW]	471.467579
Brake horsepower [kW]	471.467579
Net work required [kW]	471.467579
Power loss [kW]	0
Efficiency	0.72
Mechanical efficiency	1
Outlet pressure [bar]	11
Outlet temperature [C]	422.81062
Isentropic outlet temperature[C]	314.422948
Vapor fraction	1

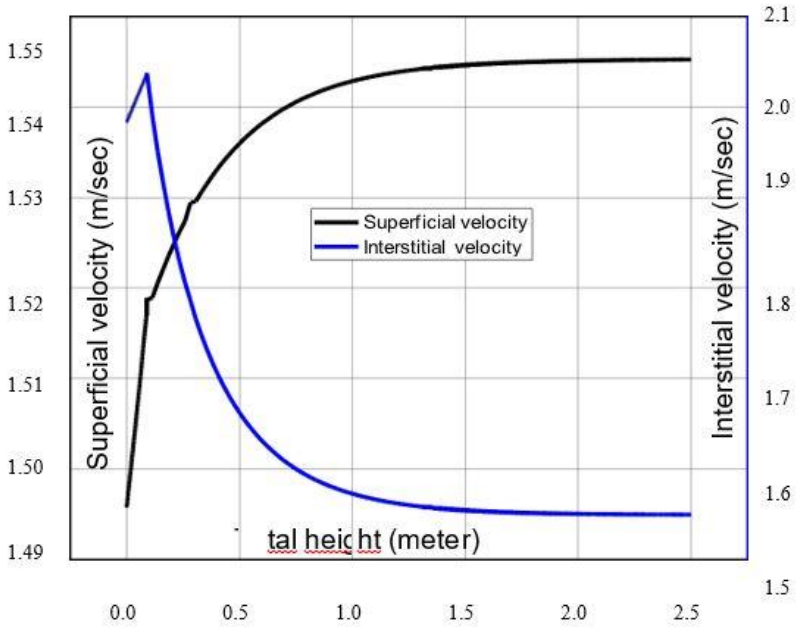


Figure-3 is indicated the superficial and interstitial velocity that varies through fluidized bed reactor column height, a black color is specified superficial velocity, while a blue color is denoted interstitial

velocity.The relationship between superficial and interstitial velocity is implemented in Aspen plus. This relationship is mathematically expressed by:

$$\text{Interstitial velocity} = \frac{\text{Superficial velocity}}{1 - \text{solid volume fraction}} \quad \text{or} \quad V_{it} = \frac{V_{su}}{1 - \varepsilon_s} \text{ ------6}$$

Where a superficial velocity is calculated by:

$$V_{su} = \frac{\text{Fluid volume flow rate}(Q)}{\text{Fluid flow area}(A)} \text{ ----------7}$$

The next figure is the result of solid volume fraction (ε_S) distribution and pressure drop along the total height of fluidized bed reactor.

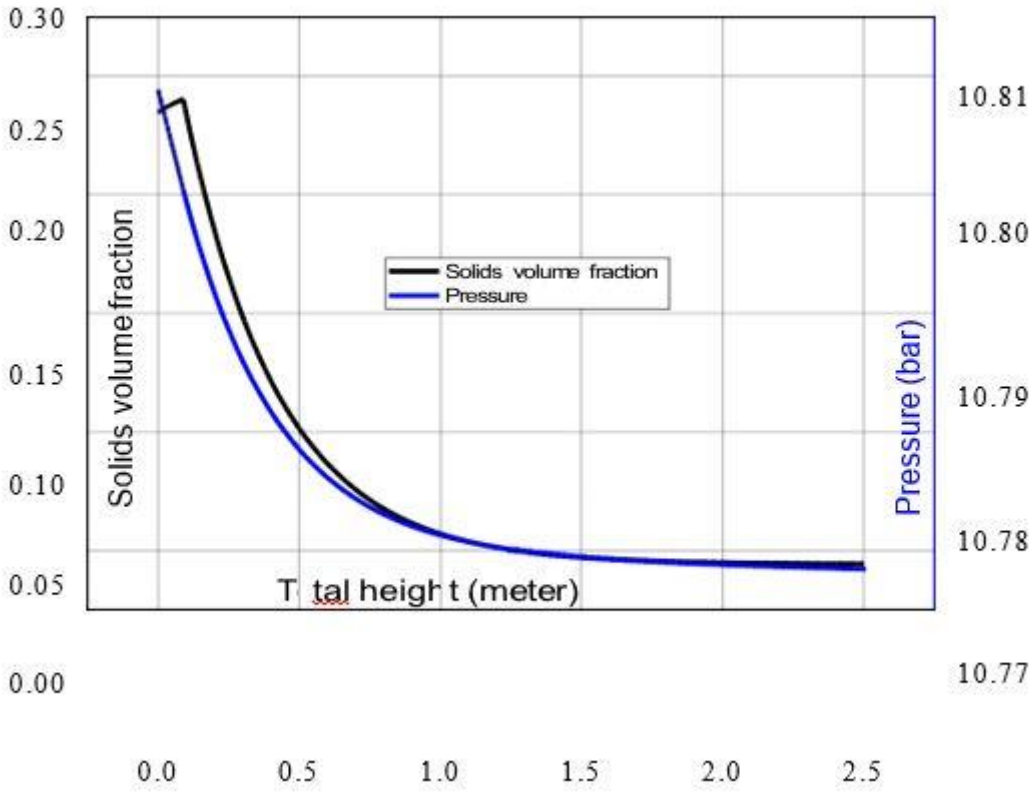


Figure-4 isthe solid volume fraction distributed and the pressure drop through in fluidized bed column after modeling and simulation was converged. As a black line on a figure is indicated at the bottom of column the bed particles are dense and exponential decreased upward to the column height. It is becoming to zero, when the column height is reached 1.5meter.So, no bed particles or catalysis in an outlet and recommended the total height of column not exceed 2.5 meter. A blue line on a figure-4 is indicated the pressure drop through the fluidized bed column, it is obtained from the converged modeling and simulation result. The pressure drop is exponentially decreased through the column due to presented bed particles and solid materials.

4. Conclusion:

The conclusion of the Aspen Plus (advanced systems processes engineering software) modeling and simulation of fluidized bed reactor for case-specific to aluminum hydroxide decomposition reaction. Mostly, the Aspen plus model predictions obtain a reasonable agreement through the experimental results. This modeling and simulation are used Geldart B particle classification within Gates-Gaudin-Schuhmann for particle size distribution function. Newton parameters are applied to mass convergence and the used Ergun equation is merely applied for a minimum fluidization velocity calculation and pressure drop through the fluidized bed reactor. The main prediction of this work is to prevent catalysts or used small quantities of bed particles and identified their melting point. According to the modeling and simulation, results indicated best to choose bed particles (catalyst) temperature should be above 340°C. This fluidized bed reactor model and simulation is practical for aluminum hydroxide decomposition reaction. The feed input to the Fluidized bed is 275 kg/hr of $Al(OH)_3$mass flow rate, after the decomposition reaction take place. It is converted into (output) 169.6 kg/hr of aluminum oxide (Al_2O_3) and 89.9 kg/hr of water.

Overall, the modeling and simulation results are indicated good efficiency and 94.4% of aluminum hydroxide mass conversion.

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